David M. Rogers, Ph.D.
Computational Physical Chemist

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EDUCATION

Sandia National Laboratory, Albuquerque, New Mexico — 2009-present
Sandia Postdoctoral Researcher, Dr. Susan B. Rempe Lab
Center for Biological and Materials Sciences

University of Cincinnati, Cincinnati, Ohio — 2009
Ph.D. Physical Chemistry, Dr. Thomas L. Beck Lab
Dissertation: Using Bayes' Theorem for Free Energy Calculations

We investigated the central quantity of free energies in a Bayesian context and provide estimators for solvation free energies as well as optimal potential of mean force approximations to model polymer coarse-grained dynamics from atomistic simulations.

University of Cincinnati, Cincinnati, Ohio
B.S. Chemistry With Biochemistry Concentration — 2004
Minor: Mathematics
Honors: Cum laude

HIGHLIGHTED SKILLS

- Advising and improving student academic development – 2 sections, 6 quarters at 25 undergraduate students per class during teaching assistantship, student mentoring.
- Expanding available computational tools for free energy calculation, probability estimation, coarse-graining, and uncertainty quantification.
- Fundamental physical studies of the molecular mechanisms and energy balance of mechanical and biological systems from electronic to nanoscale resolution levels.

EXPERIENCE

Lead Developer of Computational Chemistry Software — 2004-present

Developed MMFF condensed phase MD simulations program SEA.
Designed and implemented several other analysis programs in python and C languages – Bayesian force matching, multiple structural superposition, cyclic coordinate descent, clique detection, T-WHAM solver, and various coordinate and trajectory analysis routines.

Genome Research Institute, University of Cincinnati
Unix System Administrator — 2004-2006
Installed and maintained hardware and software of several systems, including an SGI Altix running Redhat Enterprise Linux, a 10 processor Scyld 64-bit Opteron cluster, and multiple user machines running Linux. Also collaborated with OSC on maintenance of an 80 node Opteron 64-bit cluster. Performed web server maintenance during consultant work for Entegrations Inc.

Co-developer of Web Server Software for Computational Infrastructure — 2004-2006
Collaborated with developers of GRIDP project at the University of Cincinnati Genome Research Institute.

Department of Chemistry, University of Cincinnati
Lecture and Laboratory Teaching Assistant 2004-2006
Taught two recitations and two labs per quarter averaging 20 students each, collaborated on development of test materials, met with students upon request, and graded all coursework.

Dr. Beck Group, University of Cincinnati
Undergraduate Research Assistant Summer 2003
Supported laboratory activities and collaborated on multigrid research programs and strategies, coded and parallelized PNP solver using MPI.

GRANTS

- Sandia Laboratory LDRD in collaboration with the MD Anderson Cancer Center, Understanding Conformational Changes in Asparaginase Enzyme Function 2010
- Department of Energy Computational Science Graduate Fellowship DE-FG02-97ER25308 2006-2009
- Department of Chemistry Teaching Assistantship and University Graduate Scholarship 2004-2006

PUBLICATIONS

- **David M. Rogers**, Thomas L. Beck, and Susan B. Rempe. "Information Theory Perspective on Nonlinear, Nonequilibrium Thermodynamics." arXiv:1105.5662v1, *J. Stat. Phys. in press,* 2011.

  We show how the interpretation of thermodynamic states as representing system information leads naturally to thermodynamic cycles and the first and second laws of thermodynamics as well as similar formulations for nontrivial nonequilibrium problems. The logical development of the theory also leads naturally to correct indistinguishability factors in the partition function.

- Sameer Varma, **David M. Rogers**, Lawrence R. Pratt, and Susan B. Rempe. "Perspectives on Ion Selectivity: Design Principles for K^+ Selectivity in Membrane Transport." *J. Gen. Physiol., 137(6):479-488,* 2011.

  We review the development of models for understanding the physical basis of selectivity for K^+ ions over Na^+, its sibling only one row behind, in membrane channels and transporters. Although the problem is subtle because of the morass of competing effects, we emphasize work analyzing the systematic influence of the environment on tipping local binding site structure toward selective configurations.

- **David M. Rogers** and Susan B. Rempe. "A First and Second Law for Nonequilibrium Thermodynamics: Maximum Entropy Derivation of the Fluctuation-Dissipation Theorem and Entropy Production Functionals Applicable to Arbitrary Thermal and Mechanical Processes." arXiv:1105.5619v1 *submitted to Phys. Rev. E,* 2011.

  A complete theory for classical statistical mechanics of driven systems is presented. The maximum entropy formalism carries over to transient and time-dependent processes and identifies the Green-Kubo relations as generalized Gibbs relations.

- **David M. Rogers** and Susan B. Rempe. "Thermodynamic Analysis of Nanoporous Membrane Separation Devices" *manuscript in progress*, 2011.

  This paper discusses the cross-over between molecular dynamics and nonequilibrium hydrostatics approximations and derives an energy efficiency analysis for desalination membranes in the local equilibrium limit.

- Susan B. Rempe and **David M. Rogers**; et. al. "Computational and experimental platform for understanding and optimizing water flux and salt rejection in nanoporous membranes." *Sandia Technical Report*, SAND2010-6735, 2010.

  We summarize work on designing polymer coatings for salt exclusion in water transporting nanopores. In this work, I collected available molecular dynamics results for these systems and performed a novel energy efficiency analysis able to relate atomistic and experimental scales as well as identify important

design goals and chemical principles for material performance.

- **David M. Rogers** and Susan B. Rempe. “Probing the Thermodynamics of Competitive Ion Binding Using Minimum Energy Structures.” *J. Phys. Chem. B*, 115(29):9116-9129, 2011.

  We presented an extension of the quasi-chemical theory for quantifying the impact of structure on ion complexation thermodynamics. The theory can be simply represented using a set of thermodynamic cycles involving binding site structural and compositional states as reaction intermediates.

- **David M. Rogers** and Thomas L. Beck. "Resolution and Scale Independent Nonparametric Function Matching Using a String Energy Penalized Spline Prior." arXiv:1003.4741v1 [stat.ML], to be submitted for peer review.

  Fresh insight is provided into long-standing mathematical issues surrounding computational modeling of continuous functions from a few sampled data points. The present research lays the groundwork for predicting the behavior of complicated many-body systems using advanced regression techniques.

- Zhen Zhao, **David M. Rogers** and Thomas L. Beck. “Polarization and Charge Transfer in the Hydration of Chloride Ions.” *J. Chem. Phys.*, 132:014502, 2010.

  Dr. Zhao's *ab-initio* analysis of the charge distribution in water-ion clusters highlighted the importance of many-body water-water interactions and charge transfer effects in determining cluster structural and energetic properties. These are still challenging to represent in modern polarizable forcefields and have implications for anion properties at interfaces.

- **David M. Rogers** and Thomas L. Beck. “Quasi-Chemical and Structural Analysis of Polarizable Anion Hydration.” *J. Chem. Phys.*, 132:014505, 2010.

  The role of polarizability in forcefield-based models of ions and water was examined. Utilizing some of our recent developments on quasi-chemical theory, we have been able to quantify the tightened, asymmetric nature of the ion's local solvation waters induced by increased polarizability as well as the exact effects of polarization on the solvation free energy. The results suggest some potential problems and diagnostics for such models.

- David M. Rogers and Thomas L. Beck. Force Solve (Sourceforge, Chicago IL, 2008).

  This force matching software uses somewhere above 4000 lines of code to implement and test coarse-graining for general molecular systems. It is able to parametrize coarse Hamiltonians from atomic trajectory data given arbitrary definitions of coarse united-atom type models as well as carry out short Langevin Dynamics simulations on the coarse scale. The program's main drawbacks are its slow speed and high memory usage due to its simplistic design.

- David M. Rogers and Thomas L. Beck. "Modeling Molecular and Ionic Absolute Solvation Free Energies with Quasi-Chemical Theory Bounds." *J. Chem. Phys.* 129:134505, 2008.

  Ions disrupt the local solvent structure in complicated ways, making a chemically accurate calculation of their transfer free energies difficult. Several key modeling issues encountered in applying quasi-chemical theory to gain insight into this problem were resolved.

PRESENTATIONS

- Conference on Computational Physics, Gatlinburg, July 2011.
- Invited Presentation, Materials Design in Chemical Compound Space, “Organizing Desalination Membrane Design Using Thermodynamic Cycles,” Institute for Pure and Applied Mathematics, UCLA, May 2011.
- American Physical Society March Meeting, Dallas, “Thermodynamic Analysis of Nanoporous Membrane Separation Processes”, 2011.
- Invited Presentation, Telluride Science Research Center Workshop, “Probing the Thermodynamics of Ion Hydration Using Minimum Energy Structures,” July 2010.
- Invited Presentation, Central Regional Meeting of the American Chemical Society. "Accurate Solvation Free Energy Computation." May 2007.
- Poster Presentation, Oesper Symposium, University of Cincinnati. “Methods for Structural Sampling of Multiple Interacting Molecules.” October 2006.
- Eric Franz, Daniel A. Rogers, David M. Rogers, and Matthew Wortman.

Ohio Supercomputer Center workshop. “Genome Research Institute Discovery Platform (GRIDP) beta testing project.” June 2006.

- Poster Presentation, Graduate Poster Forum, University of Cincinnati. “Conformational Analysis Techniques and The Protein Folding Problem.” March 2005.

HONORS AND AWARDS

- R&D100 Award, Biomimetic Membranes for Water Purification 2011
- Award for Excellence, Laboratory Directed Research & Development, Sandia 2010
- Hans H. Jaffé Award for Outstanding Scholarship in Physical Chemistry 2009
- Phi Beta Kappa, University of Cincinnati 2004
- Biochemistry Award for Graduating Senior with Most Potential 2004
  Department of Chemistry, University of Cincinnati
- McMicken Achievers Scholarship, University of Cincinnati 2003
- Deans List, University of Cincinnati 2001 – 2004

STUDENTS MENTORED

- Nathanial Musin, Undergraduate, U. Cincinnati 2007
- Kevin Kerian, Undergraduate, Western Kentucky U. (NSF REU) Summer, 2009
- Hyundeok Song, Entering Graduate Student, U. Cincinnati 2008
- Blake Baird, Entering Graduate Student, U. Cincinnati 2010
- Marielle Soniat, Graduate Student, U. New Orleans Summer, 2011

SOCIETIES

- Phi Beta Kappa, 2004-
- American Chemical Society, 2004-
- American Physical Society, 2010-